



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:30 AM UTC

PDB ID : 9OBN / pdb_00009obn
Title : Crystal structure of malaria transmission-blocking antigen Pfs48/45 C-terminal domain in complex with nanobody B2
Authors : Lyons, F.M.T.; Dietrich, M.H.; Tham, W.H.
Deposited on : 2025-04-22
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

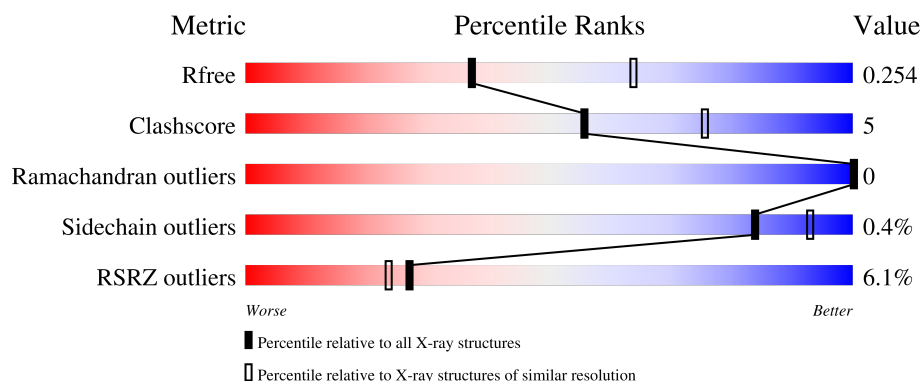
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	150	3% 83% 11% 6%
1	B	150	5% 77% 15% 9%
1	C	150	6% 84% 7% 9%
1	D	150	17% 80% 9% 11%
2	E	131	3% 89% 11%

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Mol	Chain	Length	Quality of chain
2	F	131	 3% 84% 12% .
2	G	131	 6% 82% 15% ..
2	H	131	 2% 88% 9% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gametocyte surface protein P45/48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1066	677	165	217	7			
1	B	137	Total	C	N	O	S	0	0	0
			1028	653	160	208	7			
1	C	136	Total	C	N	O	S	0	0	0
			1029	652	160	210	7			
1	D	134	Total	C	N	O	S	0	0	0
			993	628	154	204	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	GLU	-	expression tag	UNP Q8I6T1
A	289	THR	-	expression tag	UNP Q8I6T1
A	290	GLY	-	expression tag	UNP Q8I6T1
A	308	TYR	HIS	engineered mutation	UNP Q8I6T1
A	397	LEU	GLY	engineered mutation	UNP Q8I6T1
A	402	VAL	ILE	engineered mutation	UNP Q8I6T1
A	429	GLY	-	expression tag	UNP Q8I6T1
A	430	GLY	-	expression tag	UNP Q8I6T1
A	431	SER	-	expression tag	UNP Q8I6T1
A	432	GLU	-	expression tag	UNP Q8I6T1
A	433	ASN	-	expression tag	UNP Q8I6T1
A	434	LEU	-	expression tag	UNP Q8I6T1
A	435	TYR	-	expression tag	UNP Q8I6T1
A	436	PHE	-	expression tag	UNP Q8I6T1
A	437	GLN	-	expression tag	UNP Q8I6T1
B	288	GLU	-	expression tag	UNP Q8I6T1
B	289	THR	-	expression tag	UNP Q8I6T1
B	290	GLY	-	expression tag	UNP Q8I6T1
B	308	TYR	HIS	engineered mutation	UNP Q8I6T1
B	397	LEU	GLY	engineered mutation	UNP Q8I6T1
B	402	VAL	ILE	engineered mutation	UNP Q8I6T1

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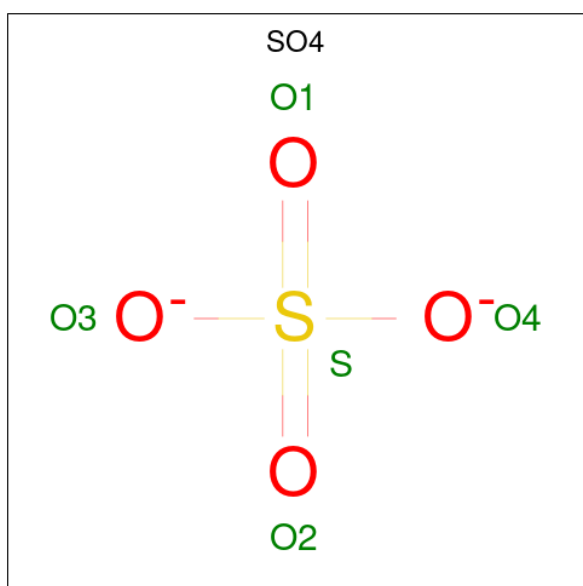
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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	GLY	-	expression tag	UNP Q8I6T1
B	430	GLY	-	expression tag	UNP Q8I6T1
B	431	SER	-	expression tag	UNP Q8I6T1
B	432	GLU	-	expression tag	UNP Q8I6T1
B	433	ASN	-	expression tag	UNP Q8I6T1
B	434	LEU	-	expression tag	UNP Q8I6T1
B	435	TYR	-	expression tag	UNP Q8I6T1
B	436	PHE	-	expression tag	UNP Q8I6T1
B	437	GLN	-	expression tag	UNP Q8I6T1
C	288	GLU	-	expression tag	UNP Q8I6T1
C	289	THR	-	expression tag	UNP Q8I6T1
C	290	GLY	-	expression tag	UNP Q8I6T1
C	308	TYR	HIS	engineered mutation	UNP Q8I6T1
C	397	LEU	GLY	engineered mutation	UNP Q8I6T1
C	402	VAL	ILE	engineered mutation	UNP Q8I6T1
C	429	GLY	-	expression tag	UNP Q8I6T1
C	430	GLY	-	expression tag	UNP Q8I6T1
C	431	SER	-	expression tag	UNP Q8I6T1
C	432	GLU	-	expression tag	UNP Q8I6T1
C	433	ASN	-	expression tag	UNP Q8I6T1
C	434	LEU	-	expression tag	UNP Q8I6T1
C	435	TYR	-	expression tag	UNP Q8I6T1
C	436	PHE	-	expression tag	UNP Q8I6T1
C	437	GLN	-	expression tag	UNP Q8I6T1
D	288	GLU	-	expression tag	UNP Q8I6T1
D	289	THR	-	expression tag	UNP Q8I6T1
D	290	GLY	-	expression tag	UNP Q8I6T1
D	308	TYR	HIS	engineered mutation	UNP Q8I6T1
D	397	LEU	GLY	engineered mutation	UNP Q8I6T1
D	402	VAL	ILE	engineered mutation	UNP Q8I6T1
D	429	GLY	-	expression tag	UNP Q8I6T1
D	430	GLY	-	expression tag	UNP Q8I6T1
D	431	SER	-	expression tag	UNP Q8I6T1
D	432	GLU	-	expression tag	UNP Q8I6T1
D	433	ASN	-	expression tag	UNP Q8I6T1
D	434	LEU	-	expression tag	UNP Q8I6T1
D	435	TYR	-	expression tag	UNP Q8I6T1
D	436	PHE	-	expression tag	UNP Q8I6T1
D	437	GLN	-	expression tag	UNP Q8I6T1

- Molecule 2 is a protein called Nanobody B2.

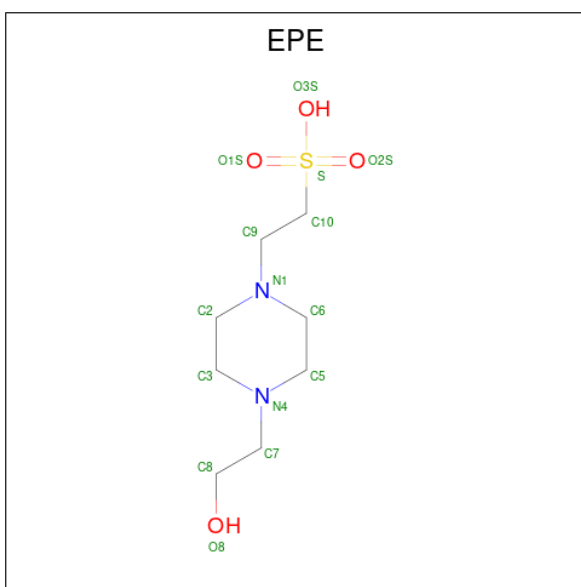
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	131	Total	C	N	O	S	0	0	0
			973	607	178	183	5			
2	H	127	Total	C	N	O	S	0	1	0
			936	585	165	181	5			
2	G	128	Total	C	N	O	S	0	0	0
			932	580	167	180	5			
2	F	126	Total	C	N	O	S	0	0	0
			922	578	162	177	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

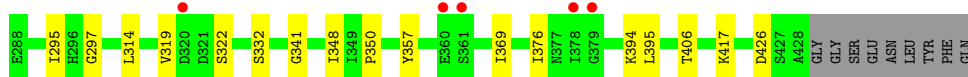
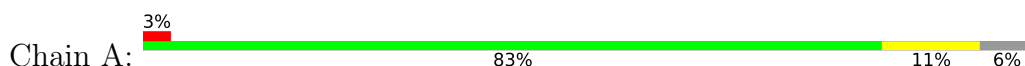
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	38	Total	O	0	0
			38	38		
5	C	64	Total	O	0	0
			64	64		
5	D	25	Total	O	0	0
			25	25		
5	E	52	Total	O	0	0
			52	52		
5	H	50	Total	O	0	0
			50	50		
5	G	54	Total	O	0	0
			54	54		
5	F	50	Total	O	0	0
			50	50		

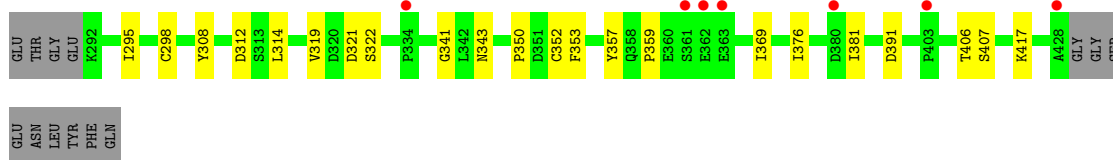
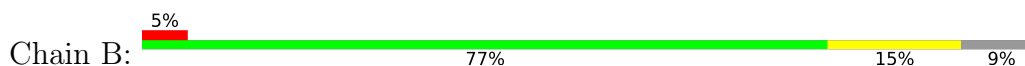
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

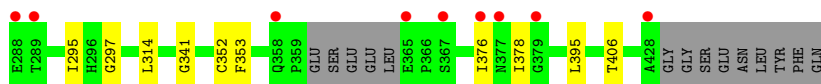
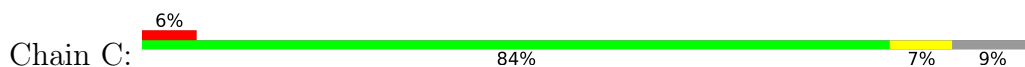
- Molecule 1: Gametocyte surface protein P45/48



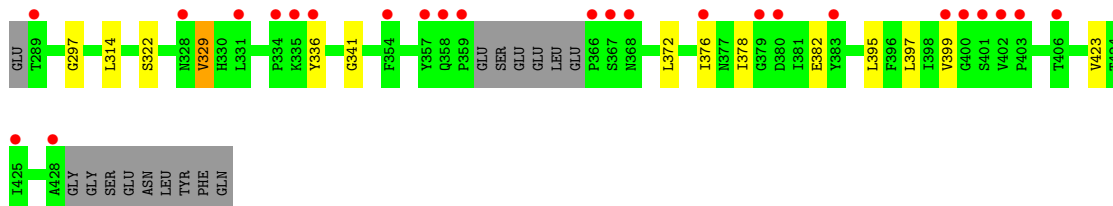
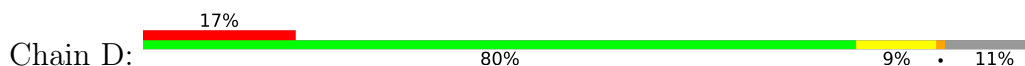
- Molecule 1: Gametocyte surface protein P45/48



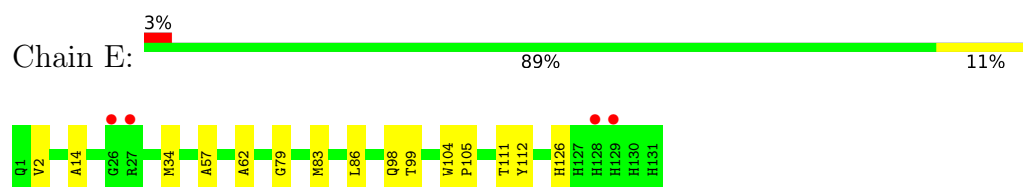
- Molecule 1: Gametocyte surface protein P45/48



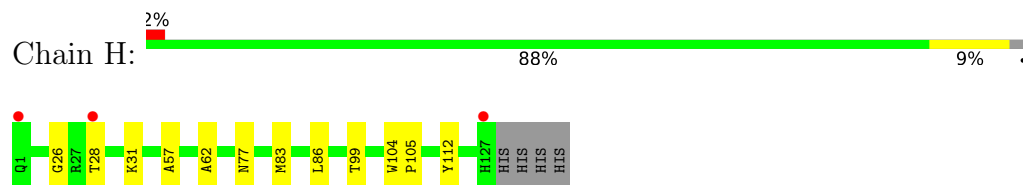
- Molecule 1: Gametocyte surface protein P45/48



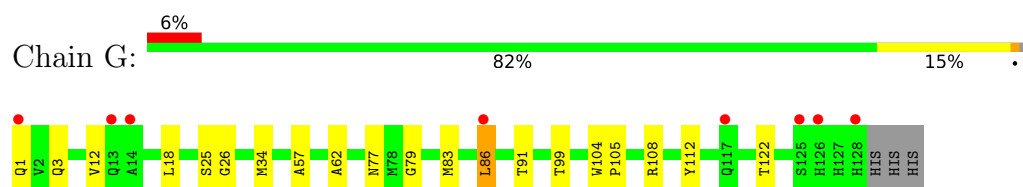
- Molecule 2: Nanobody B2



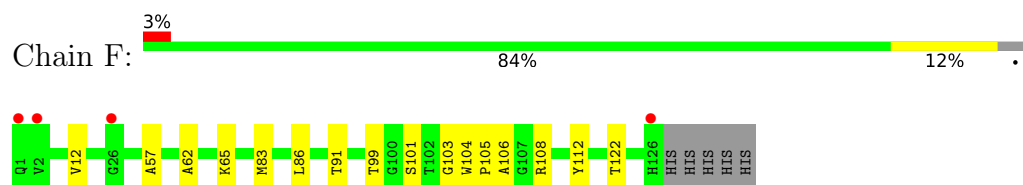
- Molecule 2: Nanobody B2



- Molecule 2: Nanobody B2



- Molecule 2: Nanobody B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.69Å 88.52Å 281.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.50 47.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.54-2.50) 99.8 (47.54-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.208 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	2124 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8302	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/1088	0.40	0/1481
1	B	0.18	0/1050	0.41	0/1433
1	C	0.16	0/1050	0.38	0/1430
1	D	0.14	0/1013	0.35	0/1381
2	E	0.18	0/999	0.36	0/1356
2	F	0.15	0/944	0.36	0/1281
2	G	0.16	0/954	0.38	0/1296
2	H	0.14	0/958	0.33	0/1300
All	All	0.17	0/8056	0.37	0/10958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1066	0	986	11	0
1	B	1028	0	943	15	0
1	C	1029	0	955	6	0
1	D	993	0	893	9	0
2	E	973	0	898	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	922	0	858	10	0
2	G	932	0	857	12	0
2	H	936	0	868	7	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	E	15	0	17	1	0
4	F	15	0	17	2	0
5	A	50	0	0	0	0
5	B	38	0	0	0	1
5	C	64	0	0	0	1
5	D	25	0	0	0	0
5	E	52	0	0	0	0
5	F	50	0	0	0	0
5	G	54	0	0	2	2
5	H	50	0	0	0	0
All	All	8302	0	7292	71	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:62:ALA:HA	2:F:65:LYS:HD3	1.57	0.87
1:A:319:VAL:O	1:A:417:LYS:NZ	2.20	0.70
2:E:14:ALA:HB3	2:E:126:HIS:HB2	1.79	0.65
1:B:314:LEU:HD12	2:E:57:ALA:HB1	1.80	0.64
1:B:319:VAL:O	1:B:417:LYS:NZ	2.29	0.63
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.82	0.61
2:E:111:THR:HG23	4:E:202:EPE:H21	1.82	0.60
2:G:1:GLN:NE2	5:G:202:HOH:O	2.32	0.60
2:E:83:MET:HE2	2:E:86:LEU:HD21	1.86	0.58
2:G:26:GLY:O	2:G:77:ASN:ND2	2.38	0.57
2:G:99:THR:HB	2:G:112:TYR:HA	1.86	0.56
1:B:376:ILE:HG13	1:B:406:THR:HG21	1.88	0.56
1:A:376:ILE:HG22	1:A:406:THR:HG21	1.89	0.55
1:B:321:ASP:OD1	1:B:417:LYS:HE2	2.07	0.55
1:C:376:ILE:HG22	1:C:406:THR:HG21	1.89	0.54
2:E:2:VAL:HG11	2:E:98:GLN:HE21	1.72	0.54
2:E:99:THR:HB	2:E:112:TYR:HA	1.89	0.54
2:G:108:ARG:NH1	5:G:205:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:HD12	2:H:57:ALA:HB1	1.90	0.53
2:H:28:THR:O	2:H:31:LYS:HG2	2.10	0.52
1:A:314:LEU:HD12	2:G:57:ALA:HB1	1.92	0.51
1:A:369:ILE:HB	1:B:369:ILE:HB	1.92	0.51
1:A:332:SER:OG	1:A:426:ASP:OD2	2.26	0.51
2:F:106:ALA:O	2:F:108:ARG:NH1	2.44	0.51
2:F:99:THR:HB	2:F:112:TYR:HA	1.93	0.51
2:G:34:MET:SD	2:G:79:GLY:HA3	2.51	0.50
1:B:376:ILE:HG21	1:B:381:ILE:HD11	1.92	0.50
1:A:322:SER:HB2	2:G:62:ALA:HB2	1.94	0.50
2:H:99:THR:HB	2:H:112:TYR:HA	1.93	0.50
1:D:382:GLU:HB2	1:D:397:LEU:HB3	1.94	0.49
1:D:376:ILE:HG13	1:D:378:ILE:H	1.78	0.49
1:B:359:PRO:HG3	1:B:407:SER:HB2	1.95	0.48
1:B:295:ILE:HD11	1:B:308:TYR:CD1	2.49	0.48
2:F:12:VAL:HG11	2:F:86:LEU:HD13	1.94	0.48
2:F:101:SER:OG	4:F:201:EPE:H101	2.14	0.47
2:G:83:MET:HB3	2:G:86:LEU:HD11	1.97	0.47
2:G:91:THR:HG23	2:G:122:THR:HA	1.96	0.47
2:F:103:GLY:HA3	4:F:201:EPE:H22	1.97	0.47
2:F:83:MET:HE2	2:F:86:LEU:HD21	1.98	0.46
2:E:34:MET:SD	2:E:79:GLY:HA3	2.56	0.46
1:B:319:VAL:HG22	2:E:105:PRO:HB2	1.98	0.46
1:C:314:LEU:HD12	2:F:57:ALA:HB1	1.98	0.45
1:D:329:VAL:HG13	1:D:423:VAL:HA	1.97	0.45
1:A:319:VAL:C	1:A:417:LYS:HZ1	2.15	0.45
1:A:297:GLY:HA3	1:A:341:GLY:O	2.17	0.45
2:G:3:GLN:HB3	2:G:25:SER:HB2	1.99	0.44
1:D:372:LEU:O	1:D:376:ILE:HG12	2.17	0.44
2:H:104:TRP:CG	2:H:105:PRO:HD3	2.53	0.44
1:B:343:ASN:OD1	1:B:391:ASP:HB3	2.18	0.44
1:D:322:SER:HB2	2:H:62:ALA:HB2	1.99	0.44
2:G:12:VAL:HG21	2:G:18:LEU:HG	2.00	0.43
1:B:350:PRO:HD3	1:B:357:TYR:CD2	2.54	0.43
1:B:341:GLY:HA2	1:B:353:PHE:CE1	2.53	0.43
1:B:298:CYS:HA	1:B:312:ASP:O	2.18	0.42
1:B:322:SER:HB2	2:E:62:ALA:HB2	2.01	0.42
1:C:297:GLY:HA3	1:C:341:GLY:O	2.19	0.42
2:H:26:GLY:O	2:H:77:ASN:ND2	2.53	0.42
2:F:91:THR:HG23	2:F:122:THR:HA	2.01	0.42
1:D:297:GLY:HA3	1:D:341:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD13	1:A:394:LYS:HG3	2.01	0.41
1:C:341:GLY:HA3	1:C:395:LEU:HD23	2.02	0.41
2:F:104:TRP:CG	2:F:105:PRO:HD3	2.56	0.41
1:D:341:GLY:HA3	1:D:395:LEU:HD23	2.03	0.41
2:E:104:TRP:N	2:E:105:PRO:HD2	2.36	0.41
1:A:350:PRO:HD3	1:A:357:TYR:CD2	2.56	0.41
1:C:295:ILE:HG21	1:C:395:LEU:HD22	2.02	0.41
1:C:352:CYS:HA	1:C:353:PHE:HA	1.83	0.41
1:A:295:ILE:HG21	1:A:395:LEU:HD22	2.03	0.41
1:D:336:TYR:O	1:D:399:VAL:HA	2.21	0.40
1:B:352:CYS:HA	1:B:353:PHE:HA	1.83	0.40
2:G:104:TRP:CG	2:G:105:PRO:HD3	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:518:HOH:O	5:G:205:HOH:O[3_454]	2.11	0.09
5:C:546:HOH:O	5:G:247:HOH:O[3_554]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/150 (93%)	134 (96%)	5 (4%)	0	100	100
1	B	135/150 (90%)	130 (96%)	5 (4%)	0	100	100
1	C	132/150 (88%)	127 (96%)	5 (4%)	0	100	100
1	D	130/150 (87%)	123 (95%)	7 (5%)	0	100	100
2	E	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
2	F	124/131 (95%)	124 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	126/131 (96%)	124 (98%)	2 (2%)	0	100	100
2	H	126/131 (96%)	126 (100%)	0	0	100	100
All	All	1041/1124 (93%)	1016 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/137 (86%)	118 (100%)	0	100	100
1	B	114/137 (83%)	114 (100%)	0	100	100
1	C	117/137 (85%)	116 (99%)	1 (1%)	70	87
1	D	108/137 (79%)	107 (99%)	1 (1%)	70	87
2	E	92/98 (94%)	92 (100%)	0	100	100
2	F	86/98 (88%)	86 (100%)	0	100	100
2	G	87/98 (89%)	86 (99%)	1 (1%)	65	84
2	H	88/98 (90%)	88 (100%)	0	100	100
All	All	810/940 (86%)	807 (100%)	3 (0%)	84	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	378	ILE
1	D	329	VAL
2	G	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS

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Mol	Chain	Res	Type
1	A	328	ASN
1	A	355	GLN
1	B	337	ASN
1	B	355	GLN
1	C	355	GLN
2	E	77	ASN
2	E	98	GLN
2	E	120	GLN
2	E	130	HIS
2	H	77	ASN
2	G	82	GLN
2	G	84	ASN
2	G	120	GLN
2	F	98	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	E	202	-	15,15,15	0.95	1 (6%)	19,20,20	1.61	4 (21%)
3	SO4	D	501	-	4,4,4	0.30	0	6,6,6	0.09	0
4	EPE	F	201	-	15,15,15	0.97	1 (6%)	19,20,20	1.96	5 (26%)
3	SO4	E	201	-	4,4,4	0.22	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	E	202	-	-	3/9/19/19	0/1/1/1
4	EPE	F	201	-	-	3/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	202	EPE	C10-S	3.19	1.82	1.77
4	F	201	EPE	C10-S	2.97	1.81	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	EPE	C5-N4-C3	4.67	118.91	108.84
4	F	201	EPE	C7-N4-C3	3.95	121.77	111.24
4	E	202	EPE	C7-N4-C3	3.04	119.35	111.24
4	E	202	EPE	C5-N4-C3	3.04	115.40	108.84
4	E	202	EPE	O1S-S-C10	3.01	111.28	106.73
4	F	201	EPE	C7-N4-C5	3.01	119.27	111.24
4	E	202	EPE	C7-N4-C5	2.88	118.92	111.24
4	F	201	EPE	C6-N1-C2	2.67	114.59	108.84
4	F	201	EPE	O2S-S-C10	2.15	109.98	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	202	EPE	S-C10-C9-N1
4	F	201	EPE	S-C10-C9-N1
4	E	202	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
4	E	202	EPE	C9-C10-S-O2S
4	F	201	EPE	C10-C9-N1-C6
4	F	201	EPE	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	202	EPE	1	0
4	F	201	EPE	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	141/150 (94%)	0.27	5 (3%)	47	42	27, 39, 66, 93	0
1	B	137/150 (91%)	0.61	7 (5%)	33	29	32, 49, 72, 93	0
1	C	136/150 (90%)	0.24	9 (6%)	24	21	28, 41, 64, 80	0
1	D	134/150 (89%)	1.06	25 (18%)	3	2	38, 59, 88, 99	0
2	E	131/131 (100%)	0.11	4 (3%)	51	47	26, 34, 63, 74	0
2	F	126/131 (96%)	0.17	4 (3%)	50	46	30, 41, 60, 81	0
2	G	128/131 (97%)	0.33	8 (6%)	26	23	27, 41, 67, 82	0
2	H	127/131 (96%)	0.15	3 (2%)	59	55	18, 39, 64, 87	1 (0%)
All	All	1060/1124 (94%)	0.37	65 (6%)	27	23	18, 42, 76, 99	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ALA	4.1
1	A	361	SER	3.6
1	D	380	ASP	3.6
1	D	367	SER	3.4
2	G	126	HIS	3.3
1	D	366	PRO	3.3
1	C	365	GLU	3.3
1	D	359	PRO	3.2
1	A	379	GLY	3.2
2	G	1	GLN	3.2
1	D	368	ASN	3.2
2	F	126	HIS	3.2
1	D	428	ALA	3.1
1	D	354	PHE	2.9
1	D	379	GLY	2.8
2	E	26	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	376	ILE	2.8
1	D	358	GLN	2.7
1	A	320	ASP	2.7
1	B	380	ASP	2.6
1	B	362	GLU	2.6
2	G	86	LEU	2.6
1	C	367	SER	2.6
1	D	334	PRO	2.6
1	D	401	SER	2.5
2	G	125	SER	2.5
1	D	335	LYS	2.5
1	D	376	ILE	2.4
2	H	28	THR	2.4
1	D	402	VAL	2.4
1	C	428	ALA	2.4
1	A	378	ILE	2.4
1	D	425	ILE	2.4
2	E	129	HIS	2.4
1	B	361	SER	2.3
1	C	358	GLN	2.3
1	B	334	PRO	2.3
1	B	363	GLU	2.3
1	D	399	VAL	2.3
2	H	1	GLN	2.3
2	H	127	HIS	2.3
2	G	128	HIS	2.3
2	G	14	ALA	2.2
1	D	406	THR	2.2
2	E	27	ARG	2.2
1	C	289	THR	2.2
1	D	331	LEU	2.2
1	D	400	GLY	2.2
2	F	26	GLY	2.2
1	B	403	PRO	2.2
1	D	289	THR	2.1
1	C	288	GLU	2.1
2	F	2	VAL	2.1
2	G	13	GLN	2.1
2	F	1	GLN	2.1
1	D	403	PRO	2.1
1	D	328	ASN	2.1
1	C	379	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	2.1
1	D	357	TYR	2.1
2	E	128	HIS	2.1
2	G	117	GLN	2.0
1	D	336	TYR	2.0
1	C	377	ASN	2.0
1	D	383	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EPE	E	202	15/15	0.72	0.19	29,43,71,86	0
4	EPE	F	201	15/15	0.79	0.24	32,41,64,73	15
3	SO4	D	501	5/5	0.83	0.08	79,80,88,128	0
3	SO4	E	201	5/5	0.95	0.09	45,55,62,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.